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MODELING OF SUBSTRATE SURFACE TEMPERATURE DISTRIBUTION
DURING HOT FILAMENT ASSISTED DIAMOND DEPOSITION

K. Tankala, T. DebRoy, W. A. Yarbrough and C. J. Robinson

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DIAMOND AND RELATED MATERIALS

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MODELING OF SUBSTRATE SURFACE TEMPERATURE DISTRIBUTION
DURING HOT FILAMENT ASSISTED DIAMOND DEPOSITION

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ABSTRACT

The importance of substrate temperature in determining the quality, uniformity and growth rate of diamond films is now well recognized. In the hot filament assisted chemical vapor deposition of diamond, the mechanism of heat transfer is unique. In addition to conduction, convection and radiation, filament to substrate heat transfer takes place by dissociation of molecular hydrogen at or near the filament and recombination of atomic hydrogen at the substrate surface. In this paper, the role of atomic hydrogen recombination in heat transfer is examined. Furthermore, the effects of system geometry and process variables on the substrate temperature distribution are analyzed. The results indicate that atomic hydrogen recombination at the substrate plays a significant role in substrate heating. In hot filament assisted diamond deposition, system geometry, filament temperature and pressure are the most important factors in determining the substrate temperature distribution.

INTRODUCTION

In the last decade several low pressure diamond deposition techniques have been developed.^{1,2} Synthesis of good quality-defect free diamond films for potential optical and electronic applications is being pursued.³ Furthermore, significant progress is being made in understanding the growth mechanism⁴⁻⁶ and the formation of defects⁶⁻⁸ such as twins, dislocations, stacking faults, second phase inclusions and interstitial hydrogen. Essentially single phase diamond films can be deposited from hydrocarbon-hydrogen mixtures over a narrow range of substrate temperatures⁹ with significant co-deposition of amorphous carbon at lower temperatures, and formation of non-diamond components including micro-crystalline graphite at higher temperatures.¹⁰ The incorporation of defects in the diamond lattice is believed to originate from the differences in the relative rates of addition and incorporation of carbon atoms during film growth.⁶ Since the rates of carbon addition and incorporation are sensitive functions of temperature, understanding and control of the substrate temperature distribution is of crucial importance for the deposition of uniform quality-defect free diamond films, especially when large surface areas are to be coated.

In most materials processing systems, conduction, convection and radiation are the primary modes of heat transfer. However, in any chemical vapor deposition process involving atomic hydrogen, the mechanism of heat transfer is unique. The formation of atomic hydrogen at or near the filament surface is highly endothermic. Atomic hydrogen readily recombines on solid surfaces to form molecular hydrogen and the reaction is highly exothermic. Thus, in hot filament systems, atomic hydrogen acts as a heat carrier from the filament to the growth surface in addition to the conventional modes of heat transport. In much of the previous work the roles of atomic hydrogen in gas phase chemistry,¹¹ gas-surface reactions and growth mechanism⁴⁻⁶ were investigated. However, none of the previous work was aimed at understanding the role of atomic hydrogen in affecting the substrate temperature distribution.

Since the quality, morphology and defect density of the diamond films are sensitive to temperature, a uniform surface temperature is crucial for the deposition of diamond films with uniform properties. Thus, the heat transfer to the substrate and the resultant substrate temperature distribution are important considerations in the design of

reactors for coating large areas. Furthermore, a knowledge of the various factors that have a substantial influence on the substrate temperature distribution is crucial for reactor design and scale-up. None of the previous work was aimed at determining the effects of reactor geometry and process parameters on the substrate temperature distribution. Experimental determination of the surface temperature distribution is a difficult task. A recourse is to model the filament to substrate heat transfer in the reactor, so that the effects of system geometry and process variables on the temperature distribution can be examined.

In this paper the role of atomic hydrogen recombination in heat transfer and the effects of system geometry and process variables on the substrate temperature distribution are examined. The computational task involved the solution of a set of partial differential equations for the conservation of momentum, enthalpy and concentration of hydrogen atoms. The model accounts for substrate heating due to exothermic recombination of atomic hydrogen on the substrate surface in addition to heat transfer by conduction, convection and radiation. The velocity, temperature and atomic hydrogen concentration fields for an existing reactor are determined to examine the mechanisms of heat and mass transfer and to understand the factors influencing the substrate temperature distribution.

PROCEDURE

The heat transfer and fluid flow in an existing bell jar type HFCVD reactor was modeled to examine the various factors that influence the substrate temperature distribution. The bell jar reactor modeled in this study included a silicon substrate placed on a water cooled copper block. The silicon wafer was 25 mm in diameter and 3.2 mm in thickness. The copper block was 25 mm in thickness and 100 mm in diameter. The filament(s) were placed at a distance of 3 to 10 mm from the substrate. Typically, the separation between the filaments was 6.5 mm. Experiments were conducted under various filament spacings, filament-to-substrate distances, filament temperatures and reactor pressures at a constant hydrogen flow rate of 1000 sccm ($1.6 \times 10^{-5} \text{ m}^3/\text{s}$). The temperature at the top edge of the copper block was measured in each case with a thermocouple. In all experiments, the cooling water supply rate was kept constant and the changes in the inlet water temperature during the course of the experiments were

insignificant.

The heat transfer and fluid flow phenomena in the HFCVD reactor are represented by equations of the following form for the conservation of momentum, enthalpy and concentration¹² of hydrogen atoms.

$$\frac{\partial}{\partial x_i} (\rho u_i \phi) = \frac{\partial}{\partial x_i} \left[\Gamma \frac{\partial \phi}{\partial x_i} \right] + S \quad (1)$$

where ρ is the density, u_i is the component of velocity in the i direction, ϕ is the dependent variable which can represent velocity components, temperature or concentration of hydrogen atoms, S is the volumetric source term, and Γ is the diffusion coefficient which is given an appropriate meaning depending on the variable considered. The specific equations are described in standard texts^{12,13} and are not presented here. The contributions of radiation and chemical heating effects are incorporated into the calculations by defining appropriate source terms.

Figure 1 shows the computational domain. The domain represents a vertical half-section of the bell jar reactor bound by the axis of the reactor on the left and the reactor wall on the right. Since the system is symmetric about a plane passing through the axis of the reactor, only half a section of the reactor was considered to minimize the computational task. The calculations were performed for a two-dimensional, steady state, laminar flow case considering constant values of density, viscosity, thermal conductivity, specific heat and diffusion coefficient. An average temperature between the filament and the inlet gas temperatures was used for the estimation of thermophysical values unless otherwise mentioned. The data used for the calculations are presented in Table I. The input to the model included the size and shape of the reactor and its contents, the thermophysical properties, the rate of supply and the composition of the inlet gas mixture, and the heating conditions. The velocity, temperature and atomic hydrogen concentration fields were obtained from the calculations. The boundary conditions included prescription of the input velocity distribution at the top of the reactor based on the total gas flow rate. The temperature of the inlet gas stream was prescribed to be the room temperature. At the axis of the reactor, the velocity, temperature and hydrogen atom concentration gradients were taken to be zero on the basis of the symmetry consideration. At the walls of the reactor and at all solid sur-

faces the velocities were assumed to be zero on the basis of the no-slip condition. the reactor walls, the temperature was prescribed to be the room temperature and the hydrogen atom concentration was taken to be negligible. At the exit end, the velocity, temperature and atomic hydrogen concentration fields were assumed to be fully developed. An appropriate heat transfer coefficient was specified at the walls of the copper block to account for water cooling. The equations were represented in a finite difference form and solved iteratively^{12,14} on a line-by-line basis. A nonuniform grid spacing was used for obtaining maximum advantage in the resolution of variables. The computed temperatures at the top edge of the copper block, at location T in Figure 1, were compared with the experimentally measured values at various filament temperatures. Figure 2 shows that the predicted temperatures at the monitoring location are in good agreement with the corresponding experimental values and fall well within the range of experimental error. Thus, the model can be used as a reliable tool to examine the effects of system geometry and process parameters on the substrate temperature distribution.

RESULTS AND DISCUSSION

The velocity and temperature fields, computed for typical diamond deposition conditions, were used to examine the primary mechanisms of heat and mass transfer in the gas phase. In the region between the substrate and the filaments, the convective velocities were of the order of 10^{-3} m/s as can be observed from Figure 3(a). At these velocities it takes approximately 3 seconds for the various species generated at or near the filament surface to travel from the filament to the substrate placed 3 mm away. Since the time constants for the loss of some of the important species such as CH_3 and H are of the order of a millisecond, the species generated at the filament cannot be transported to the growth surface by convective mass transport. The relative importance of mass transport by convection and diffusion can be examined by the Peclet number for mass transfer, Pe . The Peclet number is defined as the ratio of convective mass transfer to diffusive mass transfer and is given by uL/D , where u is the average velocity, D is the diffusion coefficient and L is a characteristic length for the system defined as the filament to substrate distance. An order of magnitude calculation of the Peclet number for this system yields a value of 10^{-4} indicating diffusion, and not convection.

to be the dominant mechanism of mass transport. DebRoy et al^{15,16} presented experimental evidence which indicates that in typical hot filament reactors for diamond deposition, diffusion is the primary mechanism of mass transfer. Thus, the low value of Peclet number for this system is consistent with experimental observations.

Figure 3(b) shows the temperature field in the HFCVD reactor at a typical gas flow rate of 1000 sccm ($1.6 \times 10^{-5} \text{ m}^3/\text{s}$). If convection were a significant mode of heat transfer, a change in the gas flow rate should result in a substantial change in the temperature field. However, when the gas flow rate was varied from 100 to 2000 sccm (1.6×10^{-6} to $3.3 \times 10^{-5} \text{ m}^3/\text{s}$) the temperature field did not change significantly. This indicates that convection is unimportant in determining the temperature distribution and that conduction is the primary factor in establishing the temperature field. The ratio of the convective heat transport to conductive heat transport, the Peclet number for heat transfer, is given by $\rho u L C_p / k$, where L is the characteristic length for the system, u is the average velocity and ρ , C_p and k are the density, specific heat and thermal conductivity of the gas respectively. For this system, the Peclet number for heat transfer is also of the order of 10^{-4} . Thus, the insignificant influence of flow rate on the temperature field is consistent with the low value of Peclet number, and indicates that conduction, and not convection, is the dominant mechanism of heat transfer in the gas phase.

The computed atomic hydrogen concentration profiles in the reactor are presented in Figure 4. In calculating the concentration fields, an equilibrium concentration of atomic hydrogen was assumed to prevail at the filament. In addition, a large proportion of atomic hydrogen is assumed to recombine to form molecular hydrogen at the substrate surface. Figure 4(a) shows the atomic hydrogen concentration profiles in the reactor. The values of the contours represent atomic hydrogen concentrations as fractions of its concentration at the filament. Since the value of the Peclet number for mass transfer is very small the concentration field is established primarily by diffusion and convection does not play any significant role in determining the local atomic hydrogen concentrations in the reactor. Figure 4(b) shows that in the region between the filament and the substrate, the concentration profiles are not exactly parallel to the substrate surface indicating that the flux of atomic hydrogen at the substrate surface

is spatially nonuniform. Thus, the hydrogen recombination effect is spatially nonuniform, and can contribute to significant spatial variations of temperatures at the substrate surface.

In hot filament systems, where the filament is heated in excess of 2250 K, significant substrate heating can take place as a result of radiation from the filament. The amount of radiation from the filament intercepted by the substrate is given by $Q_{\text{rad}} = \sigma \epsilon A_s F_{\text{sf}} T_f^4$, where σ is the Stefan-Boltzmann constant, ϵ is the emissivity of the filament, A_s is the area of the substrate, F_{sf} is the view factor, and T_f is the filament temperature. The relative importance of radiation and conduction in filament to substrate heat transfer can be examined with the help of a dimensionless ratio. The ratio of heat transfer by radiation to heat transfer by conduction is given by $\sigma \epsilon T_f^3 L/k$, where L is a characteristic length defined as the filament to substrate distance and k is the thermal conductivity of the gas. An order of magnitude calculation of this dimensionless ratio yields a value of about 4 indicating that the radiation heat transfer is significantly more important than the conduction heat transfer. We have previously shown that the change in substrate temperature with reactor pressure was negligible.¹⁷ This finding shows that the conduction heat transfer is unimportant.

In order to determine whether heating due to atomic hydrogen recombination at the substrate surface is important, substrate temperature profiles were computed for helium and hydrogen atmospheres. Figure 5 shows the calculated substrate temperature distribution in helium and hydrogen. The temperature distribution in helium is a result of the heat transfer to the substrate by conduction, convection and radiation. If these mechanisms were the only means of heat transfer from the filament to the substrate, the substrate temperature in hydrogen should not be substantially different from that in helium. However, under identical conditions of filament temperature, reactor pressure, gas flow rate and system geometry, the calculated substrate temperature in hydrogen was much higher than that in helium. Thus, the heat generated by the recombination reaction



makes a significant contribution to substrate heating.

The effects of system geometry and process variables on the substrate temperature distribution were determined. In the HFCVD reactor described above, the substrate is placed on its holder which is water cooled to maintain its temperature within acceptable limits for diamond growth.⁹ However, no special care is taken to insure a good thermal contact between the substrate and the holder. An inadequate contact offers a resistance to heat flow thus limiting the extent to which the substrate can be cooled. The effect of this thermal contact resistance between the substrate and its holder was investigated. As a first approximation, the contact resistance was assumed to be primarily due to the gas filling the crevices between the surfaces in contact. Since the actual area of contact is negligible compared to the apparent area of contact, it is assumed that an essentially continuous layer of gas, i.e. a contact gap, separates the two surfaces. An appropriate thickness for the gap has been considered to be the sum of the root-mean-square roughness values for the two surfaces in contact. It is observed from Figure 6 that the substrate temperature is sensitive to the thickness of the contact gap. Thus, by improving the contact between the substrate and its holder, the reactor can be operated with a smaller distance between the filament and the substrate without excessive heating of the sample due to radiation and chemical effects. As a result, higher growth rates can be achieved due to high concentrations of the growth species near the substrate.

The results presented in Figure 5 indicate that in this system the atomic hydrogen recombination at the substrate surface leads to only about fifty degree rise in the substrate temperature. However, earlier investigations^{17,18} show that the chemical heating effect is much more pronounced in typical HFCVD systems. The apparently small role of atomic hydrogen in the heat transfer from the filament to the substrate in this system is attributed to substantial water cooling of the substrate holder. In the presence of water cooling, the effect of heat input is substantially diminished. As a result, the substrate temperature becomes less sensitive to variations in process conditions. In order to obtain a realistic picture of the influence of various process parameters and the system geometry on the substrate temperature in conventional systems where large water cooled copper blocks are not utilized, a typical HFCVD reactor has been modeled. In the remaining section of this paper, the results obtained for a typical HFCVD reactor are discussed.

The conventional HFCVD reactor differs from the special reactor described earlier in that the substrate is placed on a graphite substrate holder with no substrate cooling and fewer than five refractory metal filaments are used. Figure 7 shows the calculated substrate temperature distributions in helium and hydrogen atmospheres for a typical HFCVD reactor. It is observed that the temperatures in hydrogen are much higher than those in helium. Thus, the recombination of atomic hydrogen is a very important factor in substrate heating.

Figure 8 indicates that the spacing between the filaments is an important factor in determining the temperature distribution. Jansen et al.¹⁹ conducted experiments to examine the effect of filament spacing on the diamond deposition. They found that the thickness uniformity of the diamond film was a sensitive function of the separation between the filaments. The filament spacing can significantly influence the spatial distribution of the nutrient species at the substrate surface and hence, the local growth rates. Figure 8 indicates that the changes in temperature distribution can also play an important role in determining the film uniformity.

Previous investigations²⁰ indicated that the growth rate of the diamond film could be significantly improved by reducing the filament-to-substrate distance. However, the enhanced growth rates were often accompanied by film nonuniformity and even graphitic deposits.²¹ The effect of filament-to-substrate distance on the substrate temperature distribution is presented in Figure 9. The results indicate that the substrate temperature can be controlled by adjusting the filament-to-substrate distance. The thickness nonuniformity and graphitic deposits obtained at small filament-to-substrate distances can be largely attributed to excessive heating of the substrate by both atomic hydrogen recombination and conventional heat transfer mechanisms, particularly radiation from the filament.

Several types of refractory metal filaments,¹⁹ viz., Ta, W, and Re, and carbon elements²² have been used to deposit diamond films over a variety of substrates. The effects of filament and substrate emissivities on the substrate temperature distribution were examined. Figure 10(a) shows that changes in substrate emissivity during nucleation and initial stages of diamond film growth may significantly alter the substrate temperature distribution. Furthermore, appropriate changes in process conditions are

required for coating substrates with different emissivities. The filament emissivity is also an important parameter in determining the temperature of the substrate, as can be observed from Figure 10(b). The use of different filament materials can result in significantly different substrate temperatures. Furthermore, changes in filament emissivity due to carburization of the filament during initial stages of the deposition can result in substantial changes in substrate surface temperature.

The effects of filament temperature and reactor pressure on substrate heating were investigated. Figure 11(a) shows the effect of filament temperature on the substrate temperature. At high filament temperatures, significant amounts of atomic hydrogen are generated at the filament which results in a large flux of atomic hydrogen at the substrate and, consequently, a high substrate temperature. In addition, the radiation heat intercepted by the substrate increases significantly with increasing temperature of the filament. Figure 11(b) shows the effect of pressure on the substrate temperature. An increase in pressure results in an increase in the concentration of atomic hydrogen at the filament. However, the diffusion coefficient of atomic hydrogen decreases linearly with pressure. Thus, the flux of atomic hydrogen at the substrate surface decreases. The smaller recombination heat associated with this reduced flux of hydrogen atoms results in lower substrate temperatures. Thus, both the filament temperature and the reactor pressure play a significant role in substrate heating while the gas flow rate is unimportant in determining the substrate temperature.

CONCLUSION

The heat transfer and the resulting substrate temperature distribution in an existing HFCVD reactor has been modeled. In addition to conduction, convection and radiation, the model accounts for heat transfer due to dissociation of molecular hydrogen at or near the filament and recombination of atomic hydrogen at the substrate surface. An evaluation of the various heat transport mechanisms indicated that atomic hydrogen recombination at the substrate surface plays a significant role in determining the substrate temperature distribution. Radiation from the filament makes a substantial contribution to the overall filament-to-substrate heat transfer. Conduction and convection are not important in the heat transfer to the substrate. Furthermore, the results indicate that in hot filament assisted chemical vapor deposition of diamond,

system geometry, reactor pressure and filament temperature are the most important factors in determining the substrate temperature distribution.

ACKNOWLEDGEMENTS

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List of Figures

Figure 1. Schematic diagram of the computational domain.

Figure 2. Comparison of the computed temperatures at the top edge of the copper block with corresponding experimentally determined values at different filament temperatures.

Figure 3. (a) Velocity and (b) temperature fields computed for typical diamond deposition conditions of 2423 K filament temperature, 100 torr pressure and 1000 sccm gas flow rate. The five filaments are placed 3 mm from the substrate and adjacent filaments are 6.5 mm apart.

Figure 4. (a) Atomic hydrogen concentration field computed for typical diamond deposition conditions presented in Figure 3. (b) Magnified view of the profiles in the region between the filaments and the substrate. The values of the profiles represent atomic hydrogen concentrations as fractions of its concentration at the filament.

Figure 5. Substrate temperature distribution in hydrogen and helium for the conditions described in Figure 3.

Figure 6. Peak substrate temperature versus contact gap thickness for the conditions presented in Figure 3.

Figure 7. Substrate temperature distribution in hydrogen and helium for a typical hot filament reactor at 2500 K filament temperature, 30 Torr pressure and 1000 sccm gas flow rate. The two filaments are placed 10 mm from the substrate and the separation between the filaments is 13 mm.

Figure 8. Substrate temperature distributions for different filament spacings at 2500 K filament temperature, 30 torr pressure, 1000 sccm gas flow rate and filament-to-substrate distance of 10 mm.

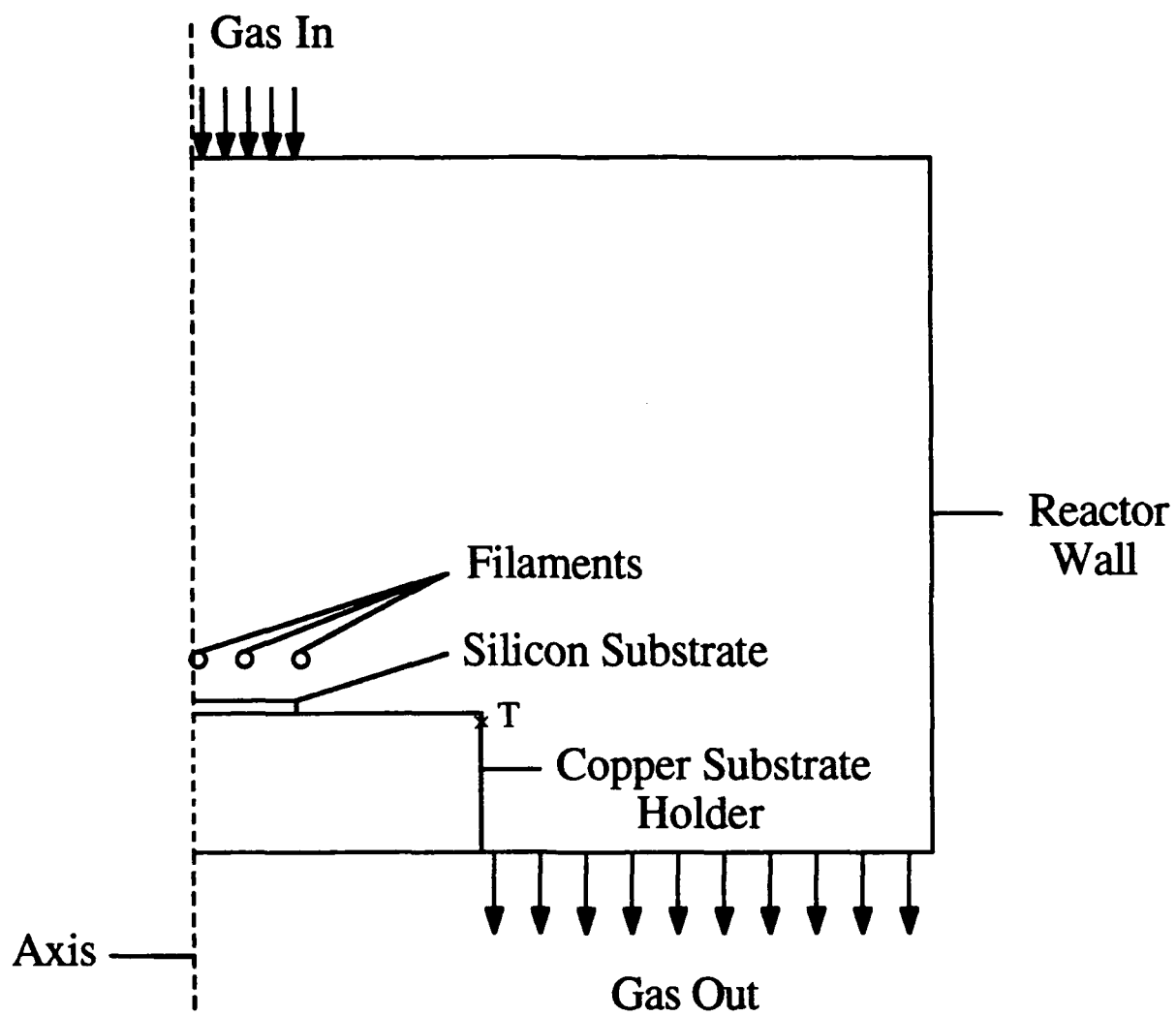
Figure 9. Peak substrate temperature versus filament-to-substrate distance at 2500 K filament temperature, 30 torr pressure, 1000 sccm gas flow rate and 13 mm separation between the two filaments.

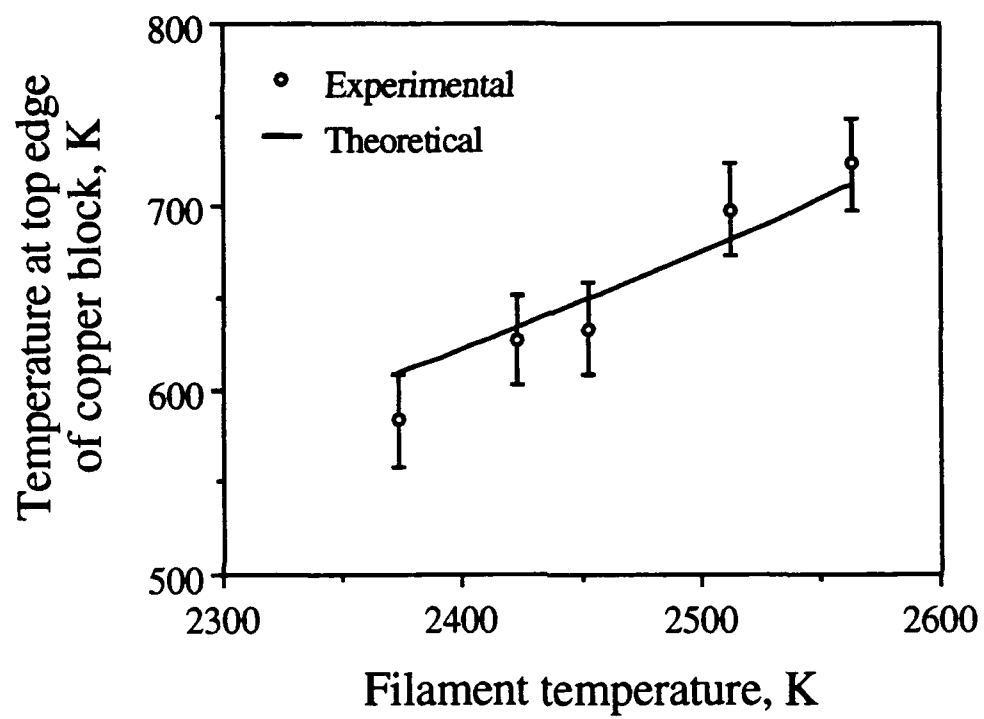
Figure 10. Peak substrate temperature versus (a) substrate emissivity and (b) filament emissivity for the conditions presented in Figure 7.

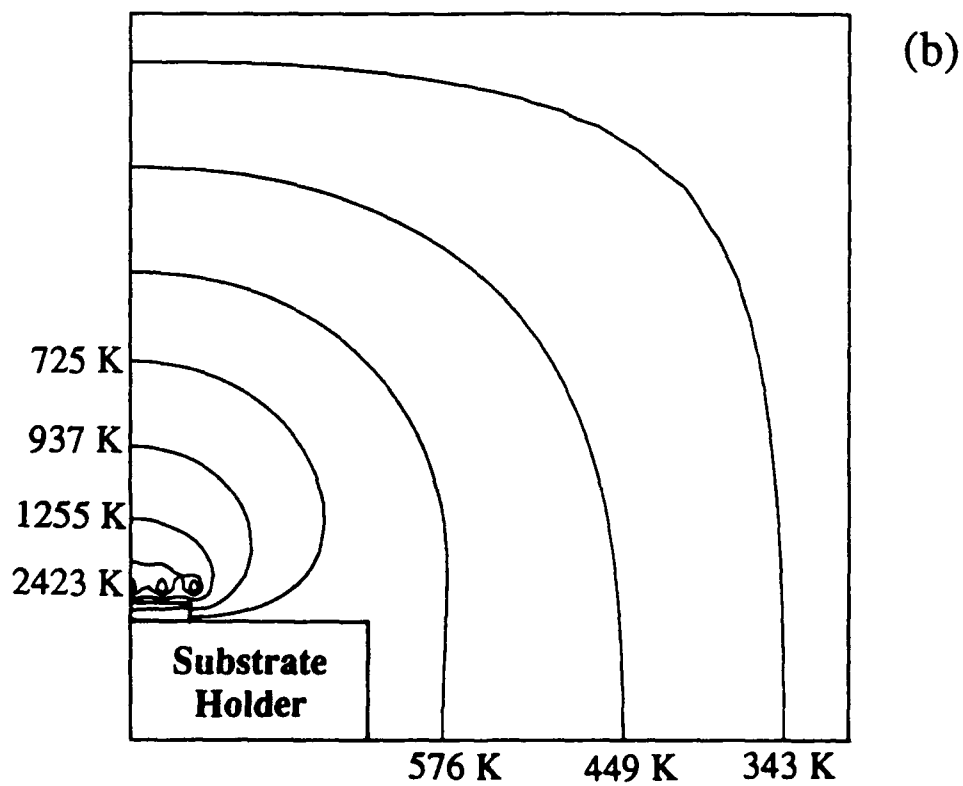
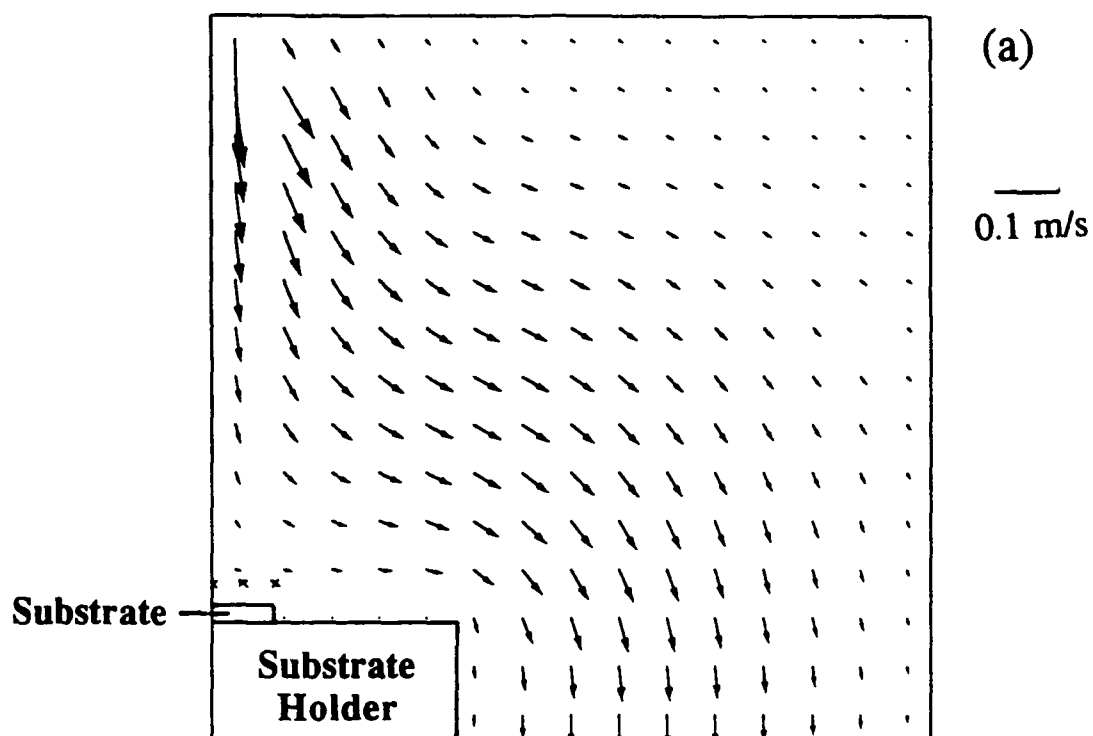
Figure 11. Variation of substrate temperature with (a) filament temperature and (b) pressure for the conditions presented in Figure 7.

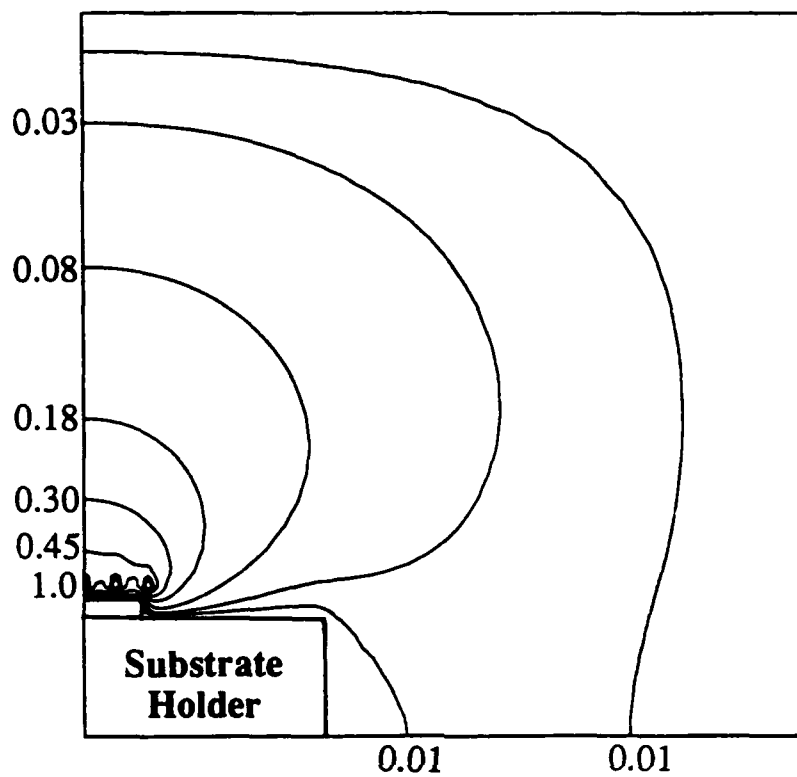
Table I Data used for calculations.

Property	Value
Thermal conductivity, W/m-K	
Hydrogen	0.525
Copper	336
Silicon	23.5
Specific heat, J/kg-K	
Hydrogen	14.05×10^{-3}
Copper	0.42×10^3
Silicon	1.02×10^3
Density, kg/m ³	
Hydrogen	2.36×10^{-3}
Copper	8.94×10^3
Silicon	2.33×10^3
Viscosity of hydrogen, kg/m-s	2.396×10^{-5}
Diffusion coefficient of H in H ₂ , m ² /s	2.82×10^{-2}
Heat transfer coefficient, W/m ² -K	693
Substrate emissivity	0.4
Filament emissivity	0.9
Contact gap, μm	40

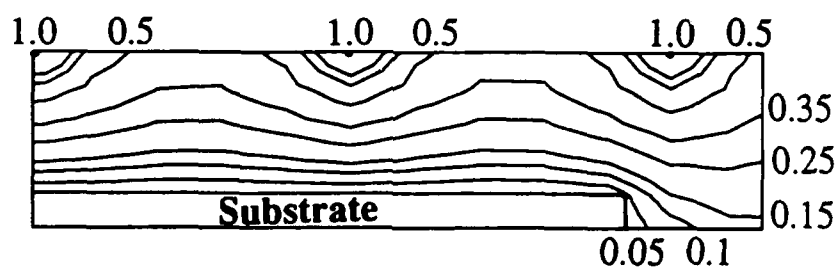




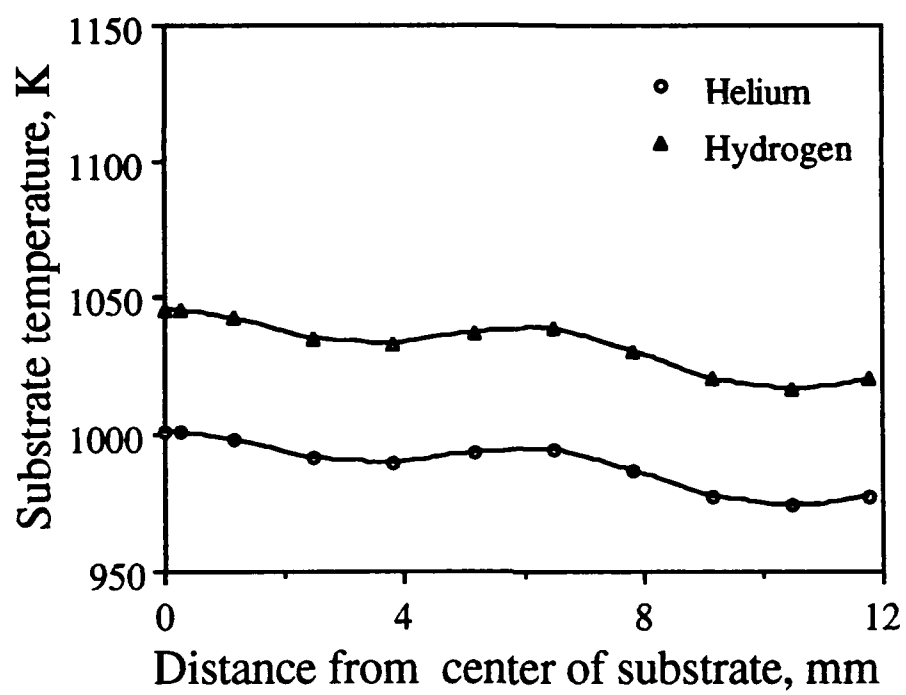


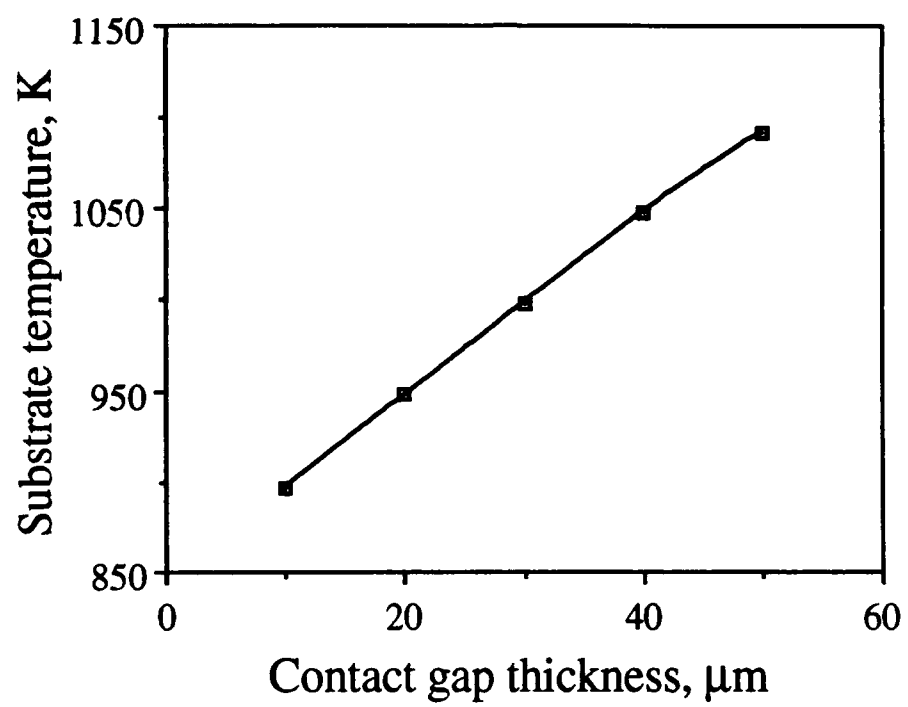


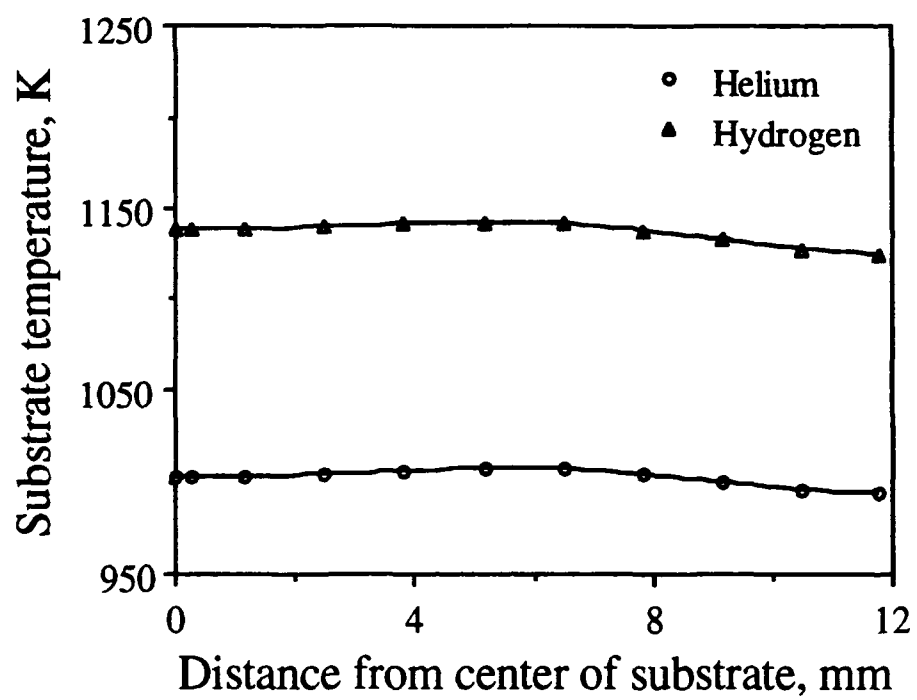
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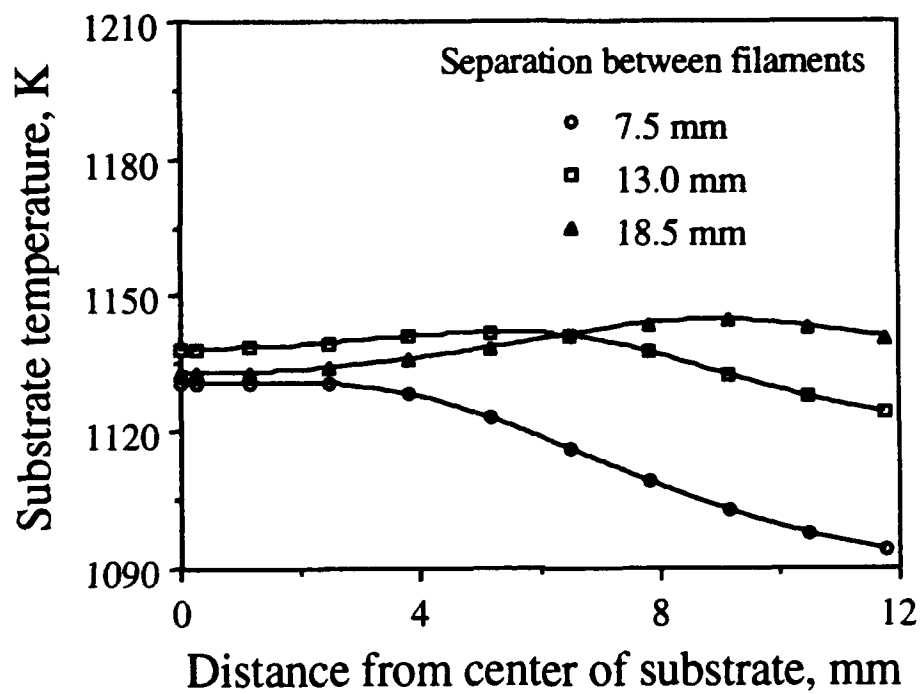


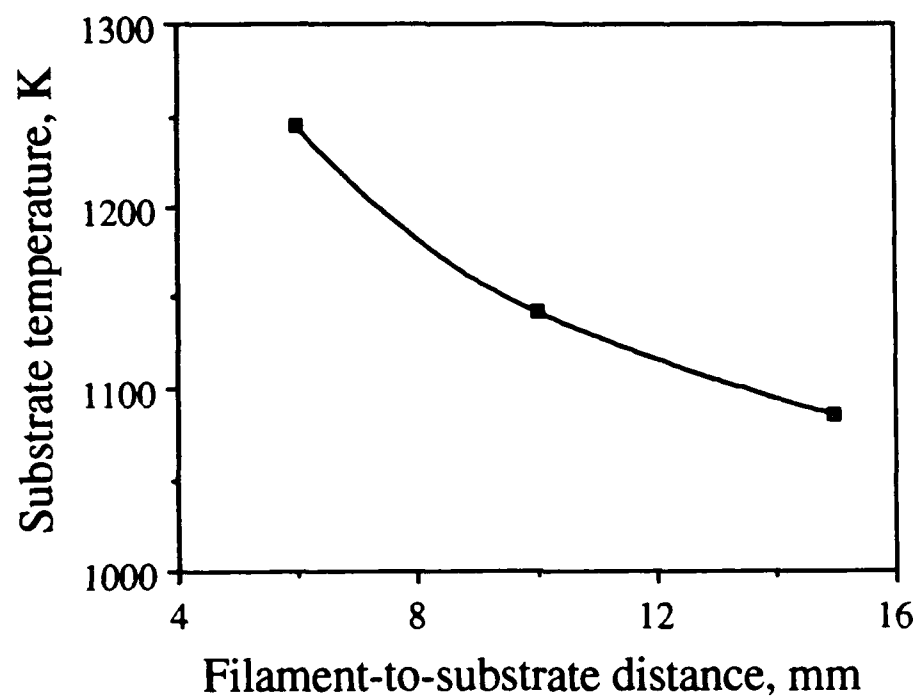
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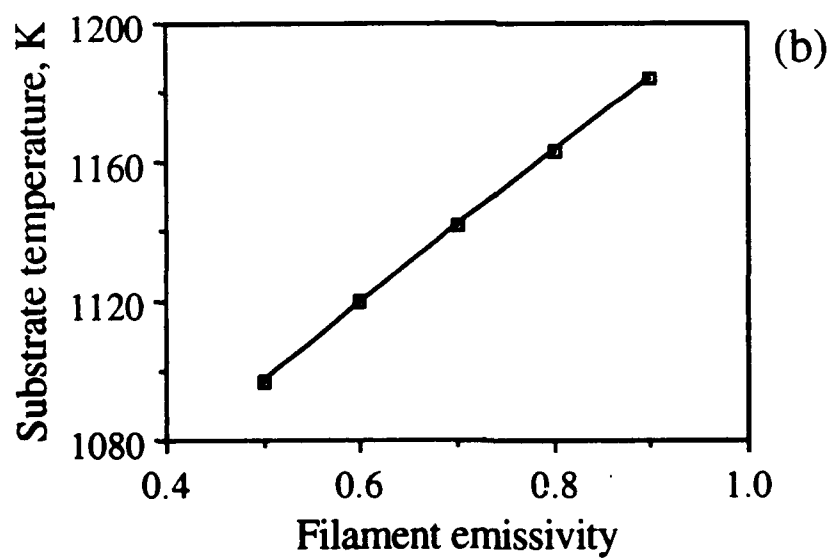
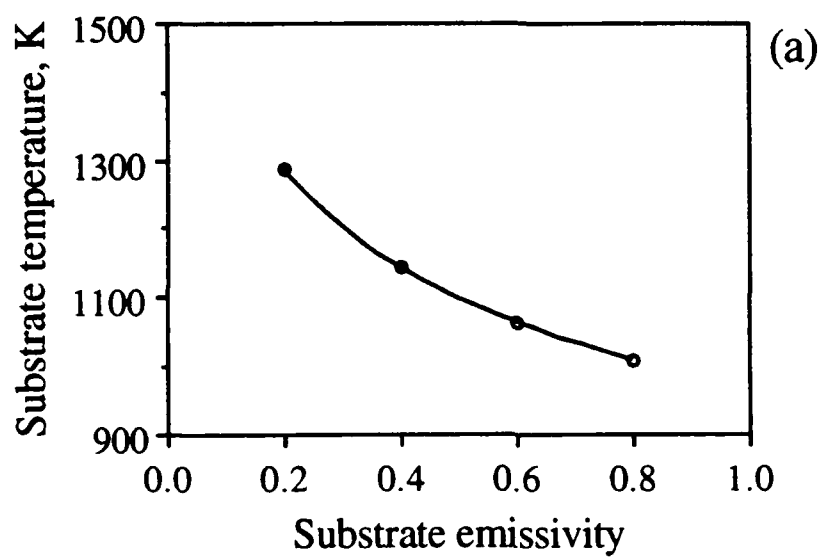


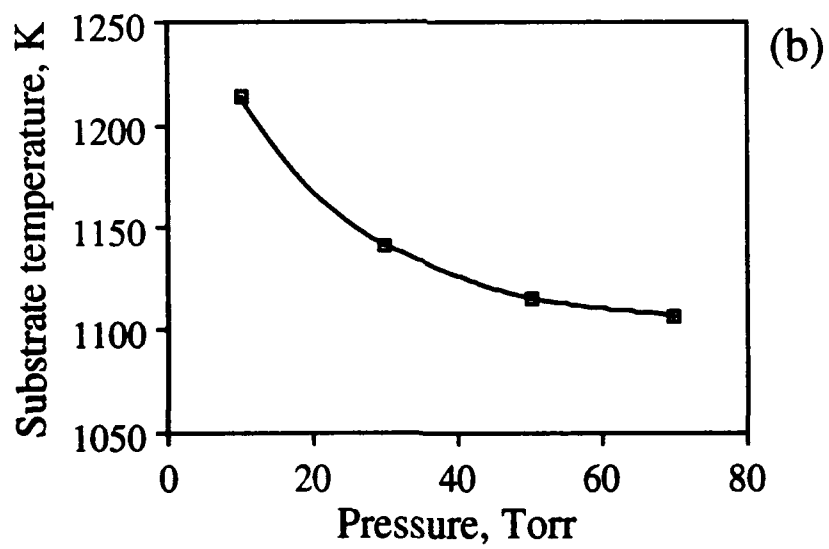
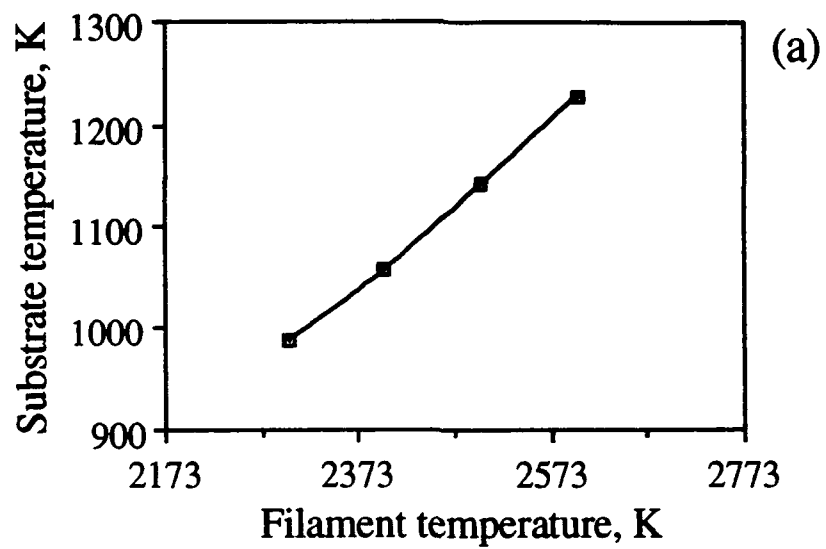












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